## Adaptive Grid Methods for Phase Field Models of Microstructure Development

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## **Project Summary**

The objective of this research program is to apply advanced numerical methods for tracking solidification phase boundaries, with the purpose of discovering the mechanisms for pattern selection during dendritic growth. We use adaptive finite element techniques to resolve the multiple length scales which arise in this problem. Before summarizing the results of our studies, we first present some introduction to provide a context.

The NASA Microgravity Science program has had a long-standing program to support the study of microstructure development in metals and transparent analog systems. The features of most interest relate to pattern selection and the evolution of length scales during solidification. These features can be strongly influenced by the presence of gravity through the interaction of the diffusion field near the solidifying crystal and buoyancy-induced convection.

Researchers have studied these phenomena using both experimental and theoretical methods. Glicksman and co-workers have made careful experiments to determine the role of various processing variables in the development of microstructures in pure succinonitrile and pivalic acid. These experiments have been performed under both microgravity and terrestrial conditions. These and other experiments result in correlations between processing variables such as undercooling and microstructural features, such as dendrite tip radius.

The theoretical study of dendritic growth has followed a parallel path to the experimental programs. The dendrite has been modeled as a parabaloid of revolution, growing at constant velocity, V. The parabaloid can be characterized by its tip radius, R. Ivantsov showed that the solution for the diffusion field around such a needle crystal growing into an undercooled melt admits an infinite number of solutions consistent with the product of VR, but that neither parameter is determined uniquely. Temkin later modified Ivantsov's treatment to include surface tension, which leads to a maximum in the infinity of possible V-R solutions. Glicksman later demonstrated that the operating state for real dendrites does not conform to this point, however. Langer,  $et\ al.$  showed that when the anisotropy of surface tension is also considered, the spectrum of solutions becomes discrete, rather than continuous, and further that only one of these solutions is stable. This is the predicted operating state for the dendrite. This latter theory is referred to as microscopic solvability.

Experimental confirmation of these theories has not yet been achieved. One difficulty is that it is not always clear that the conditions used to derive microscopic solvability theory apply during solidification of real dendrites. Real dendrites are complex-shaped entities, with a smooth tip that breaks down into sidebranches, which in turn breakdown into further sidebranches, and so on. These geometries are too complex to be examined using analytical methods. Accordingly, most recent approaches to examine dendritic growth employ numerical methods.

A promising numerical method for this purpose is the phase-field method. The singular surface of separation between the liquid and solid phases is replaced by a continuous function which varies between -1 in the liquid and +1 in the solid. The method is contrived to keep the interface where the transition occurs to be very thin – on the order of the capillary length (a material constant equal to about 10 nm). Much development has been done by many researchers over the last 10 to 15 years on this method. In particular, it has been shown that the computational grid must be smaller than the capillary length in order to ensure that the phase-field model converges to the original problem with a sharp interface.

This causes computational difficulty when the other length scales in the problem are considered. The motion of the growing crystal is controlled by the diffusion field ahead of the dendrite. The characteristic length of this diffusion field is given by D/V, where D is the diffusion coefficient. The computational domain must include several D/V for the calculation to be meaningful. For real systems, in the range of parameters where experiments can be performed, the ratio of these two length scales can be as high as 10,000. Thus, a uniform grid which correctly resolves both length scales contains a prohibitively large number of grid points. Previous researchers have avoided this difficulty by considering only large undercooling, where V is large, and hence D/V is small. Unfortunately, experiments cannot be performed in this region.

In the program, we have developed adaptive finite element methods which permit us to examine realistic, experimental conditions. The mesh is adapted to the requirements of the solution: from a very fine grid to resolve the phase-field at the interface, to a larger size appropriate for the diffusion field. The grid evolves dynamically, tracking the motion of the interface and the accompanying diffusion field. The code is written using FORTRAN 90, with dynamic memory allocation and a quadtree data structure which supports the refinement and unrefinement, as needed. We have demonstrated that the CPU-time of the code scales with the length of the interface, rather than the size of the domain.

Karma and Rappel used the phase field model to demonstrate that microscopic solvability theory applies at high undercooling. We verify our algorithm by comparing our results to repeat these calculations. The adaptive grid algorithm permits us to extend these computations to low undercooling. In this case, we found an unanticipated result: the interaction of distinct branches interferes with the growth of each arm. These results suggest that the results of microscopic solvability theory may not apply at low undercooling, except at very long times, which may explain the lack of agreement between theoretical and experimental investigations. The results of this work have been published in *Physical Review Letters* (Provatas, Goldenfeld and Dantzig, *PRL*, vol. 80, pp. 3308-3311, 1998).

We have recently performed calculations with parameters which approximate the experimental conditions used for growing pivalic acid crystals in the Isothermal Dendritic Growth Experiment (IDGE) conducted on the Fourth United States Microgravity Payload (USMP-4). We are collaborating with Prof. Glicksman and co-workers to provide a detailed comparison of the calculations and experiments. We are also working to extend our methods to consider directional solidification of alloy dendrites.